

Nitromethane
75-52-5 | DTXSID2020977

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 90.5 °C

Global applicability domain: Inside

Local applicability domain index: 6.03e-01

Confidence level: 5.06e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Nitromethane</div> <div>Measured: 101</div> <div>Predicted: 90.5</div>	<div>Image not found</div> <div>Acetaldehyde oxime</div> <div>Measured: 115</div> <div>Predicted: 110</div>	<div>Image not found</div> <div>Nitroethane</div> <div>Measured: 114</div> <div>Predicted: 117</div>
<div>Image not found</div> <div>Methyl nitrite</div> <div>Measured: -12.0</div> <div>Predicted: 17.7</div>	<div>Image not found</div> <div>Methyl isocyanate</div> <div>Measured: 39.5</div> <div>Predicted: 78.7</div>	